AN APPLICATION OF POSITIVE DEFINITE FUNCTIONS TO THE PROBLEM OF MUBS

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Abstract. We present a new approach to the problem of mutually unbiased bases (MUBs), based on positive definite functions on the unitary group. The method provides a new proof of the fact that there are at most $d+1$ MUBs in $\mathbb{C}^d$. It may also lead to a proof of non-existence of complete systems of MUBs in dimension 6 via a conjectured algebraic identity.

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1. Introduction

In this paper we present a new approach to the problem of mutually unbiased bases (MUBs) in $\mathbb{C}^d$. Our approach has been motivated by two recent results in the literature. First, in [21] one of the present authors described how the Fourier analytic formulation of Delsarte's LP bound can be applied to the problem of MUBs. Second, in [24, Theorem 2] F. M. Oliveira Filho and F. Vallentin proved a general optimization bound which can be viewed as a generalization of Delsarte's LP bound to non-commutative settings (and they applied the theorem to packing problems in Euclidean spaces). As the MUB-problem is essentially a problem over the unitary group, it is natural to combine the two ideas above. Here we present another version of the non-commutative Delsarte scheme in the spirit of [21, Lemma 2.1]. Our formulation in Theorem 2.3 below is somewhat less general than [24, Theorem 2], but makes use of the underlying group structure and is very convenient for applications. It fits the MUB-problem naturally, and leads us to consider positive definite functions on the unitary group.

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The paper is organized as follows. In the Introduction we recall some basic notions and results concerning mutually unbiased bases (MUBs). In Section 2 we describe how the problem of MUBs fits into a non-commutative version of Delsarte's scheme. We then apply this method to give a new proof of the fact that there are at most $d+1$ MUBs in $\mathbb{C}^d$. Finally, in Section 3 we speculate on how the non-existence of complete systems of MUBs could be proved in dimension 6 via an algebraic identity conjectured in [22].

Recall that two orthonormal bases in $\mathbb{C}^d$, $\mathcal{A} = \{\mathbf{e}_1, \dots, \mathbf{e}_d\}$ and $\mathcal{B} = \{\mathbf{f}_1, \dots, \mathbf{f}_d\}$ are called *unbiased* if for every $1 \le j, k \le d$, $|\langle \mathbf{e}_j, \mathbf{f}_k \rangle| = \dfrac{1}{\sqrt{d}}$. A collection $\mathcal{B}_1, \dots \mathcal{B}_m$ of orthonormal bases is said to be (pairwise) *mutually unbiased* if any two of them are unbiased. What is the maximal number of mutually unbiased bases (MUBs) in $\mathbb{C}^d$? This problem has its origins in quantum information theory, and has received considerable attention over the past decades (see e.g. [14] for a recent comprehensive survey on MUBs). The following upper bound is well-known (see e.g. [1, 3, 30]):

Theorem 1.1. *The number of mutually unbiased bases in $\mathbb{C}^d$ is less than or equal to $d+1$.*

We will give a new proof of this fact in Theorem 2.4 below. Another important result concerns the existence of complete systems of MUBs in prime-power dimensions (see e.g. [1, 11, 12, 17, 20, 30]).

Theorem 1.2. *A collection of $d+1$ mutually unbiased bases (called a complete system of MUBs) exists (and can be constructed explicitly) if the dimension d is a prime or a prime-power.*

However, if the dimension $d = p_1^{\alpha_1} \dots p_k^{\alpha_k}$ is not a prime-power, very little is known about the maximal number of MUBs. By a tensor product construction it is easy to see that there are at least $p_j^{\alpha_j} + 1$ MUBs in $\mathbb{C}^d$ where $p_j^{\alpha_j}$ is the smallest of the prime-power divisors of d. One could be tempted to conjecture the maximal number of MUBs always equals $p_j^{\alpha_j} + 1$, but this is already known to be false: for some *specific* square dimensions $d = s^2$ a construction of [29] yields more MUBs than $p_j^{\alpha_j} + 1$ (the construction is based on orthogonal Latin squares). Another important phenomenon, proved in [28], is that the maximal number of MUBs cannot be exactly d (it is either $d+1$ or strictly less than d).

The following basic problem remains open for all non-primepower dimensions:

Problem 1.3. *Does a complete system of $d+1$ mutually unbiased bases exist in $\mathbb{C}^d$ if d is not a prime-power?*

For $d = 6$ it is widely believed among researchers that the answer is negative, and the maximal number of MUBs is 3. The proof still eludes us, however, despite considerable efforts over the past decade ([3, 4, 5, 6, 18]). On the one hand, some *infinite families* of MUB-triplets in $\mathbb{C}^6$ have been constructed ([18, 31]). On the other hand, numerical evidence strongly suggests that there exist no MUB-quartets [5, 6, 8, 31]. For non-primepower dimensions other than 6 we are not aware of any conjectures as to the exact maximal number of MUBs.

It will also be important to recall the relationship between mutually unbiased bases and *complex Hadamard matrices*. A $d \times d$ matrix H is called a complex Hadamard matrix if all its entries have modulus 1 and $\frac{1}{\sqrt{d}}H$ is unitary. Given a collection of MUBs $\mathcal{B}_1, \ldots, \mathcal{B}_m$ we may regard the bases as unitary matrices $U_1, \ldots, U_m$ (with respect to some fixed orthonormal basis), and the condition of the bases being pairwise unbiased amounts to $U_i^* U_j$ being a complex Hadamard matrix scaled by a factor of $\frac{1}{\sqrt{d}}$ for all $i \neq j$. That is, $U_i^* U_j$ is a unitary matrix (which is of course automatic) whose entries are all of absolute value $\frac{1}{\sqrt{d}}$.

A complete classification of MUBs up to dimension 5 (see [7]) is based on the classification of complex Hadamard matrices (see [16]). However, the classification of complex Hadamard matrices in dimension 6 is still out of reach despite recent efforts [2, 19, 23, 26, 27].

In this paper we will use the above connection of MUBs to complex Hadamard matrices. In particular, we will describe a Delsarte scheme for non-commutative groups in Theorem 2.3, and apply it to the MUB-problem with an appropriate witness function $h(Z)$ on the unitary group $U(d)$ in Theorem 2.4.

2. Mutually unbiased bases and a non-commutative Delsarte scheme

In this section we describe a non-commutative version of Delsarte's scheme, and show how the problem of mutually unbiased bases fit into this scheme. The commutative analogue was described in [21].

Let G be a compact group, the group operation being multiplication and the unit element being denoted by 1. We will denote the normalized Haar measure on G by μ. Let a symmetric subset $A = A^{-1} \subset G$, $1 \in A$, be given. We think of A as the 'forbidden' set. We would like to determine the maximal cardinality of a set $B = \{b_1, \ldots b_m\} \subset G$ such

that all the quotients $b_j^{-1}b_k \in A^c \cup \{1\}$ (in other words, all quotients avoid the forbidden set A). When G is commutative, some well-known examples of this general scheme are present in coding theory ([13]), sphere-packings ([9]), and sets avoiding square differences in number theory ([25]). We will discuss the non-commutative case here.

Recall that the convolution of $f, g \in L^1(G)$ is defined by $f * g(x) = \int f(y)g(y^{-1}x)d\mu(y)$

Recall also the notion of positive definite functions on G. A function $h : G \to \mathbb{C}$ is called positive definite, if for any m and any collection $u_1, \dots, u_m \in G$, and $c_1, \dots, c_m \in \mathbb{C}$ we have $\sum_{i,j=1}^m h(u_i^{-1}u_j)\overline{c_i}c_j \geq 0$. When h is continuous, the following characterization is well-known.

Lemma 2.1. (cf. [15, Proposition 3.35]) *If G is a compact group, and $h : G \to \mathbb{C}$ is a continuous function, the following are equivalent.*

(i) h is of positive type, i.e.

$$\int (\tilde{f} * f)h \geq 0 \tag{1}$$

for all functions $f \in L^2(G)$ (here $\tilde{f}(x) = \overline{f(x^{-1})}$)

(ii) h is positive definite

This statement is fully contained in the more general Proposition 3.35 in [15]. In fact, for compact groups Proposition 3.35 in [15] shows that instead of $L^2(G)$ the smaller class of continuous functions $C(G)$ or the wider class of absolute integrable functions $L^1(G)$ could also be taken in (i). All these cases are equivalent, but for us it will be convenient to use $L^2(G)$ in the sequel.

We formulate another important property of positive definite functions.

Lemma 2.2. *Let G be a compact group and μ the normalized Haar measure on G. If $h : G \to \mathbb{C}$ is a continuous positive definite function then $\alpha = \int_G h d\mu \geq 0$, and for any $\alpha_0 \leq \alpha$ the function $h - \alpha_0$ is also positive definite. In other words, for any m and any collection $u_1, \dots, u_m \in G$ and $c_1, \dots, c_m \in \mathbb{C}$ we have*

$$\sum_{i,j=1}^m h(u_i^{-1}u_j)\overline{c_i}c_j \geq \alpha|\sum_{i=1}^m c_i|^2. \tag{2}$$

Proof. Let $f \in L^2(G)$ and define a linear operator $H : L^2(G) \to L^2(G)$ by

$$(Hf)(x) = \int h(x^{-1}y)f(y)\,dy.$$

As h is assumed to be positive definite, H is positive self-adjoint. Also, writing $\mathbf{1}$ for the constant one function on G we have

$$H\mathbf{1} = \alpha\mathbf{1}, \quad \langle H\mathbf{1}, \mathbf{1}\rangle = \alpha \geq 0.$$

Let us use the notation $\beta = \int f$. We have the orthogonal decomposition

$$f = \beta\mathbf{1} + f_2, \quad \text{where } f_2 \perp \mathbf{1}.$$

Using invariance of the Haar measure and exchanging the order of integrations one can easily find that

$$\langle Hf, \mathbf{1}\rangle = \int (Hf)(x)\overline{\mathbf{1}(x)}\, dx = \int h(x)\, dx \int f(y)\, dy = \alpha\beta.$$

Note that here we have used the mathematician's convention according to which the scalar product is linear in its first, and conjugate linear in its second variable. Thus $\langle Hf_2, \mathbf{1}\rangle = 0$, since

$$\beta\alpha = \langle Hf, \mathbf{1}\rangle = \langle H(\beta\mathbf{1} + f_2), \mathbf{1}\rangle = \beta\alpha + \langle Hf_2, \mathbf{1}\rangle.$$

To show that $h - \alpha$ is positive definite, we need to check that

$$\langle Hf, f\rangle - |\beta|^2\alpha \geq 0$$

for all $f \in L^2(G)$. We have

$$\langle Hf, f\rangle = \langle \beta\alpha\mathbf{1} + Hf_2, \beta\mathbf{1} + f_2\rangle = |\beta|^2\alpha + \langle Hf_2, f_2\rangle$$

since $f_2 \perp \mathbf{1}$ and $Hf_2 \perp \mathbf{1}$. Hence $\langle Hf, f\rangle - |\beta|^2\alpha = \langle Hf_2, f_2\rangle \geq 0$. □

After these preliminaries we can describe the non-commutative analogue of Delsarte's LP bound. (To the best of our knowledge the commutative version was first introduced by Delsarte in connection with binary codes with prescribed Hamming distance [13]. Another formulation of the non-commutative version is given in [24]).

Theorem 2.3. *(Non-commutative Delsarte scheme for compact groups) Let G be a compact group, μ the normalized Haar measure, and let $A = A^{-1} \subset G$, $1 \in A$, be given. Assume that there exists a positive definite function $h : G \to \mathbb{R}$ such that $h(x) \leq 0$ for all $x \in A^c$, and $\int h d\mu > 0$. Then for any $B = \{b_1, \dots b_m\} \subset G$ such that $b_j^{-1}b_k \in A^c \cup \{1\}$ the cardinality of B is bounded by $|B| \leq \frac{h(1)}{\int h d\mu}$.*

Proof. Consider

$$S = \sum_{u,v\in B} h(u^{-1}v). \tag{3}$$

On the one hand,

$$S \leq h(1)|B|, \tag{4}$$

since all the terms $u \neq v$ are non-positive by assumption.

On the other hand, applying (2) with $\alpha = \int h d\mu$, $u, v \in B$ and $c_u = c_v = 1$, we get

$$S \geq \alpha |B|^2. \tag{5}$$

Comparing the two estimates (5), (4) we obtain $|B| \leq \frac{h(1)}{\int h d\mu}$. □

The function h in the Theorem above is usually called a *witness function*.

We will now describe how the problem of mutually unbiased bases fits into this scheme. Consider the group $U(d)$ of unitary matrices, being given with respect to some fixed orthonormal basis of $\mathbb{C}^d$. Consider the set CH of complex Hadamard matrices. Following the notation of the Delsarte scheme above define $A^c = \frac{1}{\sqrt{d}} CH \subset U(d)$, i.e. let the *complement* of the forbidden set be the set of scaled complex Hadamard matrices. Then the maximal number of MUBs in $\mathbb{C}^d$ is exactly the maximal cardinality of a set $B = \{b_1, \dots b_m\} \subset U(d)$ such that all the quotients $b_j^{-1} b_k \in A^c \cup \{1\}$. After finding an appropriate witness function we can now give a new proof of the fact the number of MUBs in $\mathbb{C}^d$ cannot exceed $d+1$.

Theorem 2.4. *The function $h(Z) = -1 + \sum_{i,j=1}^d |z_{i,j}|^4$ (where $Z = (z_{i,j})_{i,j=1}^d \in U(d)$) is positive definite on $U(d)$, with $h(1) = d-1$ and $\int h = \frac{d-1}{d+1}$. Consequently, the number of MUBs in dimension d cannot exceed $d+1$.*

Proof. Consider the function $h_0(Z) = \sum_{i,j=1}^d |z_{i,j}|^4$. First we prove that h_0 is positive definite. For this, recall that the Hilbert-Schmidt inner product of matrices is defined as $\langle X, Y \rangle_{HS} = \mathrm{Tr}\,(XY^*)$, and for any vector v in a finite dimensional Hilbert space H the (scaled) projection operator P_v is defined as $P_v u = \langle u, v \rangle v$. For any two vectors $u, v \in H$ we have $|\langle u, v \rangle|^2 = \mathrm{Tr}\, P_u P_v$. Also, recall that the inner product on $H \otimes H$ is given by $\langle u_1 \otimes u_2, v_1 \otimes v_2 \rangle = \langle u_1, v_1 \rangle \langle u_2, v_2 \rangle$.

Let $U_1, \dots, U_m$ be unitary matrices, $c_1, \dots, c_m \in \mathbb{C}$, and let $\{e_1, \dots, e_d\}$ be the orthonormal basis with respect to which the matrices in $U(d)$ are given. Then

$$|\langle U_r^* U_t e_j, e_k \rangle|^4 = |\langle U_t e_j, U_r e_k \rangle|^4 = |\langle U_t e_j \otimes U_t e_j, U_r e_k \otimes U_r e_k \rangle|^2 = \mathrm{Tr}\, P_{U_t e_j \otimes U_t e_j} P_{U_r e_k \otimes U_r e_k}. \tag{6}$$

Therefore, with the notation $Q_t = \sum_{j=1}^m P_{U_t e_j \otimes U_t e_j}$ we have

$$h(U_r^* U_t) = \sum_{j,k} |\langle U_r^* U_t e_j, e_k\rangle|^4 = \operatorname{Tr} Q_t Q_r. \tag{7}$$

Finally,

$$\sum_{r,t=1}^{m} h(U_r^* U_t)\overline{c_r} c_t = \|\sum_{t=1}^{m} c_t Q_t\|_{HS}^2 \geq 0, \tag{8}$$

as desired.

It is known [10] that the integral of h_0 on $U(d)$ is $\frac{2d}{d+1}$. By applying Lemma 2.2 to h_0 with $\alpha_0 = 1 < \int h_0$ we get that h is also positive definite. Note also that h vanishes on the set $\frac{1}{\sqrt{d}}CH$ of scaled complex Hadamard matrices, $h(1) = d-1$, and $\int h = \frac{2d}{d+1} - 1 = \frac{d-1}{d+1}$. Therefore, Theorem 2.3 implies that the number of MUBs in $\mathbb{C}^d$ is less than or equal to $\frac{h(1)}{\int h} = d+1$. □

We remark here that one could consider the witness functions $h_\beta = h_0 - \beta$ for any $1 \leq \beta \leq \frac{2d}{d+1}$. All these functions satisfy the conditions of Theorem 2.3. However, an easy calculation shows that the best bound is achieved for $\beta = 1$.

3. Dimension 6

In particular, let us examine the situation in dimension $d = 6$.

The function $h(Z) - 1 + \sum_{i,j=1}^{d} |z_{i,j}|^4$ in Theorem 2.4 was a fairly natural candidate which vanishes on the set of (scaled) complex Hadamard matrices $\frac{1}{\sqrt{d}}CH$, for any d. However, for $d = 6$ we have other functions which are conjectured to vanish on $\frac{1}{\sqrt{d}}CH$. Namely, Conjecture 2.3 in [22] provides a selection of such functions. Let

$$m_1(Z) = \sum_{\pi \in S_6} \sum_{j=1}^{6} z_{\pi(1),j} z_{\pi(2),j} z_{\pi(3),j} \overline{z_{\pi(4),j} z_{\pi(5),j} z_{\pi(6),j}}, \tag{9}$$

where S_6 denotes the permutation group on 6 elements. Also, let $m_2(Z) = m_1(Z^*)$. Then m_1 and m_2 are real-valued (because each term appears with its conjugate), and they are conjectured to vanish on $\frac{1}{\sqrt{d}}CH$. This provides some natural candidates for witness functions for the MUB-problem. Namely, let $m(Z) = (m_1(Z) + m_2(Z))^2$, or $m(Z) = m_1^2(Z) + m_2^2(Z)$, or $m(Z) = (m_1(Z)m_2(Z))^2$. In all three

cases $m(I) = 0$, and $\int_{Z \in U(d)} m(Z) d\mu > 0$. Therefore, if for any $\varepsilon > 0$ the function $h(Z) + \varepsilon m(Z)$ is positive definite, we get a better bound than in Theorem 2.4, and obtain that the number of MUBs in dimension 6 is strictly less than 7, i.e. a complete system of MUBs does not exist. Unfortunately, we have not yet been able to prove that such $\varepsilon > 0$ exists for any of the functions $m(Z)$ above.

Furthermore, as the inner sum in (9) is conjectured to be zero for all $\pi \in S_6$, we may even multiply each term with $(-1)^{\operatorname{sgn} \pi}$, if we wish. This leads to other possible choices of $m(z)$.

It would also be interesting to find any analogue of Conjecture 2.3 in [22] for any dimensions other than $d = 6$.

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